MeOCH2CO2 anion

Inchi: InChI=1S/C3H6O3/c1-6-2-3(4)5/h2H2,1H3,(H,4,5)/p-1
InchiKey: RMIODHQZRUFFFF-UHFFFAOYSA-M
Formula: C3H5O3-
SMILES: COCC(=O)[O-]
Mol. weight [g/mol]: 89.07
CAS: 20758-58-1

Physical Properties

Property code	Value	Unit	Source
ean	3.67 ± 0.16	eV	NIST Webbook
log10ws	-1.97		Crippen Method
logp	-1.617		Crippen Method
mcvol	64.290	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20758581&Units=SI

Legend

ean: Electron affinity of neutral species
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.